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# The Gross-Neveu Model with Chemical Potential; An Effective Theory for Solitonic-Metallic Phase Transition in Polyacetylene?

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## Abstract

The Gross-Neveu model with chemical potential is investigated as a low-energy effective theory of polyacetylene. In particular, we focus on the abrupt change in the features of electric conductivity such as sharp rise in the Pauli paramagnetism at dopant concentration of about 6%. We will try to explain it by the finite density phase transition in the Gross-Neveu model. The thermodynamic Bethe ansatz is combined with the large- $N$  expansion to construct thermodynamics of the Gross-Neveu model. A first-order phase transition

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is found in leading order in the  $1/N$  expansion and it appears to be stable against the  $1/N$  correction. The next to leading order correction to the critical dopant concentration is explicitly calculated.

## I. WHAT IS INTERESTING IN ELECTRIC CONDUCTIVITY IN POLYACETYLENE?

In this talk we want to describe our recent works on thermodynamics of the Gross-Neveu model with chemical potential. [1,2] The physical motivation for these works comes from condensed matter physics; electric conductivity properties of doped polyacetylene. [3] In particular, we are trying to describe the abrupt change in electric conductivity properties at dopant concentration of about 6%.

Polyacetylene is a typical 1-dimensional polymer and we are particularly interested in trans-type polyacetylene. It is a fascinating material, showing variety of features of electric conductivity depending upon the dopant concentration. [3] At zero doping it is an insulator. Because of the Peierls instability an electron gas in 1 dimension is unstable against generation of charge density wave [4] which entails, in this system, an alternating distortion of the lattice. It is called dimerization in condensed-matter literatures and the ground state is doubly degenerate. As a consequence an energy gap opens above the Fermi sea which implies an insulator.

At dopant concentration up to  $\sim 6\%$  the electric conductivity grows as dopant concentration increases but the Pauli paramagnetism stays low, indicating that the charge carrier is spinless. (A note for non-condensed matter physicists; doping is a procedure of importing the impurity atoms into the material to supply extra electrons or holes into the system. The dopant concentration is defined as the number of doped electrons per carbon atom.) It is believed that electric charge is transported by the spinless charged solitons in polyacetylene in this intermediate doping region. [3] One can say that the system displays the particular type of charge-spin separation.

It appears that there is a consensus that the relevant dynamical degrees of freedom are solitons in this regime. Their existence is in fact predicted by Su, Schrieffer and Heeger in their original paper. [5] They introduced the SSH Hamiltonian to describe polyacetylene and discussed its physical implications. The spectrum of solitons in this model contains two

spinless charged solitons and two neutral solitons with spin  $1/2$ . Prior to their pioneering work it was observed by Jackiw and Rebbi [6] that in theories with fermions solitons can carry fractional fermion quantum numbers. The peculiar features of spectrum of solitons in the SSH model can be nicely explained by the phenomenon of fermion fractionization.

Then, at dopant concentration of about 6% an abrupt rise occurs in the Pauli paramagnetism while the conductivity keeps monotonically increasing. In some samples the conductivity reaches as high as that of copper. [7] It is likely that the behavior indicates a transition to a metallic phase. This is the behavior that we want to understand.

## II. THE GROSS-NEVEU MODEL AS A LOW-ENERGY EFFECTIVE THEORY OF POLYACETYLENE

Soon after the proposal of the SSH Hamiltonian, it was shown by Takayama, Lin-Liu and Maki [8] that the low-energy effective continuum theory of the SSH model is given by a 1+1 dimensional relativistic four-Fermi theory with two-flavor Dirac fermions. The Lagrangian of the model can be written by using an auxiliary field  $\sigma$  (which represents the phonon degrees of freedom) and suppressing the flavor index as

$$\mathcal{L} = \bar{\psi} i \gamma^\mu \partial_\mu \psi - \frac{1}{2} \sigma^2 - g \sigma \bar{\psi} \psi \quad (1)$$

This is nothing but the field theory model which was first investigated by Gross and Neveu [9] as an asymptotically-free renormalizable quantum field theory with many common features with quantum chromodynamics.

We would like to utilize the Gross-Neveu model with chemical potential as the effective theory for a transition from solitonic to metallic phase. If it does a good job the model should display a phase transition at a certain value of the chemical potential. Is it likely? We believe that the answer is yes. It is believed that at zero chemical potential the ground state of the model violates the discrete chiral symmetry and it is doubly degenerate. It is, of course, in accord with the dimerized ground state and is nothing but the manifestation of the Peierls

instability. Therefore, the theory admits solitons (kinks) and they are “fermion-fractionized” solitons in the sense of Jackiw and Rebbi. [6] The evidence for the chiral symmetry breaking and the doubly degenerate ground state comes from the large- $N$  approximation. [9] It is also strongly supported by the existence of consistent factorizable fermion-fermion, [10] fermion-kink and kink-kink S-matrix. [11,12]

At large enough  $\mu$ , on the other hand, we believe that the symmetry is restored. Because the Gross-Neveu model is an asymptotically free theory the fermions become non-interacting at high enough densities and are not able to support their condensate that they formed to break chiral symmetry at low densities. Therefore, it is very likely that the theory displays the phase transition at a certain fermion density or at the corresponding value of chemical potential. We note that this is in disagreement with what the soliton lattice theory predicts. [13]

### III. THE GROSS-NEVEU MODEL WITH CHEMICAL POTENTIAL; THE LARGE- $N$ LIMIT

To verify (or disprove) this conjecture and to know the order of the phase transition (if any) we examined the Gross-Neveu model with chemical potential by using the large- $N$  approximation. [1] In the leading order of  $1/N$  expansion the effective potential of the model can be obtained analytically by taking into account the effect of chemical potential. It reads:

$$\begin{aligned}
V_{eff}(\sigma) &= \frac{\sigma^2}{2N} + \frac{\sigma^2}{4N} \left[ \theta(\sigma^2 - \gamma^2) \{ \ln(\sigma^2/\sigma_0^2) - 3 \} + \theta(\gamma^2 - \sigma^2) \left\{ 2 \ln \frac{\gamma + \sqrt{\gamma^2 - \sigma^2}}{\sigma_0} - 3 \right\} \right] \\
&\quad - \frac{\gamma}{2N} \sqrt{\gamma^2 - \sigma^2} \theta(\gamma^2 - \sigma^2)
\end{aligned} \tag{2}$$

where  $\gamma = \mu\sqrt{N/\pi}$ . By analyzing the expression one can easily figure out that at  $\mu = m/\sqrt{2}$ , where  $m$  is the mass of the fundamental fermion, the theory has a triple degenerate ground states. (See Ref. 1 for details.) This is a clear signature for the first-order phase transition. One can evaluate the corresponding value of the fermion density, which can be interpreted

as dopant concentration, as

$$y_c = \frac{N}{\sqrt{2\pi}\xi}$$

where  $\xi$  is the correlation length (soliton size) measured in units of lattice constant. It is estimated as  $\xi \simeq 7$  by SSH. [5] It turns out that  $y_c = 0.064$ , very close to 6% at  $N = 2$ . Here  $N$  is the number of flavor of Dirac fermion in the effective field theory. The two flavor originates the spin degrees of freedom of the electrons in the SSH model.

#### IV. GOING BEYOND THE LARGE-N LIMIT

It is a good news that the large-N works but there arise a number of questions.

- (1) Are there any experimental evidences for the first-order phase transition?
- (2) Is the large-N approximation reliable even at  $N=2$ ?
- (3) Can the result be viewed as a robust evidence for the presence of finite density phase transition in the Gross-Neveu model?

Again a good news about (1) is that apparently there exists an experiment [14] that signals a hysteresis in the Pauli paramagnetism as a function of chemical potential; a clear signature for first-order phase transition. The result, however, seems to be neither confirmed nor refuted by the other independent experiments.

The second and the third questions are more pressing to us as theorists. Certainly we should be able to do better. As a first step toward answering these questions we have calculated the next to leading order correction to see if the first-order phase transition survives (we mean, if there are any instabilities occurring) and to compute correction to the critical dopant concentration. [2]

To carry this out, however, we had to invent a novel way of computation because the direct calculation of the effective potential at two-loop with chemical potential looks to be formidable. The method we employed is a hybrid method combining the thermodynamic Bethe ansatz (TBA) and the  $1/N$  computation at zero chemical potential.

## V. THE THERMODYNAMIC BETHE ANSATZ

The thermodynamic Bethe ansatz [15,16] is a powerful method for constructing thermodynamics of a 1 dimensional system of particles whose  $S$ -matrix elements  $S_{ab}$  are exactly calculable. The technique is particularly suited to our problem because all the  $S$ -matrix elements of the Gross-Neveu model are known. [10–12] By solving the integral equation of TBA one can, in principle, construct an exact thermodynamics of the Gross-Neveu model.

Let us restrict ourselves to the elastic (or diagonal) scattering theories in which neither inelastic nor “charge-exchange” reactions occur. [17] Following Yang and Yang [15] one can write down the integral equation for dressed energy  $\epsilon_a(\theta)$  of quanta as a function of the rapidity  $\theta$ , where the subscript  $a$  specifies the particle species. It reads,

$$T\epsilon_a(\theta) = -\mu_a + m_a \cosh \theta - iT \sum_b \int d\theta' K_{ab}(\theta - \theta') \ln [1 + e^{-\epsilon_b(\theta')}] \quad (3)$$

where the kernel  $K_{ab}(\theta)$  is defined by

$$K_{ab}(\theta) = \left(\frac{1}{2\pi i}\right) \frac{d \ln S_{ab}(\theta)}{d\theta} \quad (4)$$

Having solved the equation for  $\epsilon_a(\theta)$  the free energy density of the system can be computed as

$$f(\mu) = - \sum_a \int d\theta m_a \cosh \theta \ln [1 + e^{-\epsilon_a}] + \sum_a \mu_a D_a \quad (5)$$

where  $D_a$  denotes the number density of particle  $a$ . We note that (negative of) the first term in (5) implies the pressure  $P$  because of the thermodynamic relation  $f = \mu D - P$ . Hereafter, we consider the case of single species of particles. We argue that the approximation can be justified in the large- $N$  expansion of the Gross-Neveu model.

Since we are interested in the possibility of phase transitions at finite chemical potential we want to take zero temperature limit. It is because there is no phase transition at finite temperature in 1+1 dimensions due to the Mermin-Wagner theorem. [18] <sup>1</sup> One can show

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<sup>1</sup> One can argue in length that the the Gross-Neveu model at zero-temperature serves as a better

that by taking zero-temperature limit  $T \rightarrow 0$  with  $T\epsilon(\theta) \equiv -\tilde{\epsilon}(\theta)$  kept finite, the TBA equation for “energy density” takes the form, [19]

$$\tilde{\epsilon}(\theta) = \mu - m \cosh \theta + \int_{-B}^B d\theta' K(\theta - \theta') \tilde{\epsilon}(\theta'). \quad (6)$$

where  $B$  is determined by  $\tilde{\epsilon}(B) = 0$  and the integration region is restricted to  $\tilde{\epsilon}(B) > 0$ . Using the solution of this integral equation the pressure can be expressed in zero-temperature limit as

$$P = \left(\frac{m}{2\pi}\right) \int_{-B}^B d\theta \cosh \theta \tilde{\epsilon}(\theta) \quad (7)$$

The negative of the pressure is the relevant quantity to discuss the finite-density phase transition and to calculate the critical dopant concentration. It is related with the grand canonical partition function  $\Xi$  as  $-PL = -T \ln \Xi$ . [20] (Recall the similar relationship  $F = -T \ln Z$  between the Helmholtz free energy  $F$  and the canonical partition function  $Z$ .) The fermion number density  $n$  is then given by  $-\frac{dP}{d\mu}$ .

There are, however, obstacles both technical and conceptual. The technical problem is that the integral equation is difficult to solve analytically. But it can be done numerically. On the other hand the conceptual problem is more difficult to handle. We do not know how the phase transition can be signalled in the framework of the TBA.

## VI. THE TBA IN LEADING ORDER IN $1/N$ EXPANSION

To gain insight to this problem we have examined the question by using the  $1/N$  expansion. [2] At large  $N$  one can argue that the only relevant degrees of freedom are fundamental

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effective theory of pure sample of polyacetylene at the room temperatures. The Mermin-Wagner theorem holds because of a strict one-dimensionality of space and it is known that its prohibition becomes invalid upon turning on very tiny three-dimensionality such as infinitesimal interchain couplings. H. M. thanks Yutaka Okabe for discussion on this point.

fermions because everybody else is more massive, with the masses being proportional to  $N$ . Therefore, the single species approximation should be valid. We have found an interesting structure. In leading order of  $1/N$  expansion we have the analytic expression (2) of the effective potential of the Gross-Neveu model with chemical potential. From this we can obtain the absolute value of the ground state energy density as a function of chemical potential:

$$V_{eff} = -\frac{m^2}{4\pi} + \theta(\mu^2 - m^2) \frac{m^2}{2\pi} \left[ \ln \frac{\mu + \sqrt{\mu^2 - m^2}}{m} - \frac{\mu}{m} \sqrt{\frac{\mu^2}{m^2} - 1} \right]. \quad (8)$$

Here we have chosen the renormalization point  $\sigma_0$  so that  $\lambda \equiv g^2 N = \pi$  and then  $\sigma_0$  gives minimum of the effective potential.

On the other hand, we can compute the free energy of the model by solving the TBA equation. In leading order of  $1/N$  it is trivial to solve the equation because the kernel  $K(\theta)$  vanishes (namely,  $S = 1$ ). We obtain for (negative of) the pressure,  $-P$ , the exactly the same expression as the second term in (8). The pressure given by the TBA is normalized such that it vanishes at  $\mu = m$  and there is no way (to our knowledge) of computing it below  $\mu = m$ .

It is conceivable that the pressure  $-P(\mu)$  has additional  $\mu$ -independent contribution  $-P(0)$ . It can be interpreted as the vacuum energy density of the Gross-Neveu model. On dimensional ground it can be written as  $-P(0) = -bm^2$ , where  $b$  is a constant. While there is no way of computing  $b$  within the framework of the TBA it is calculable, at least in principle, in the  $1/N$  expansion. In the leading order it was computed by Gross and Neveu [9] and  $b = 1/4\pi$ . Together with the TBA result of  $-P(\mu)$ , it reproduces the exact expression of the free energy, i.e., the effective potential (2) obtained by the explicit  $1/N$  calculation.

This establishes our strategy of how to compute free energy of the Gross-Neveu model order by order in  $1/N$  expansion. Namely, we obtain  $-P(\mu)$  by solving the TBA equation and supplement it by the vacuum energy density calculated at zero chemical potential.

Then, the question is how the TBA free energy can signal the phase transition? We propose to take massless limit of the pressure  $-P(\mu) - P(0)$  calculated by the above method

to obtain the pressure in the massless phase. [2] We have

$$-P_{massless}(\mu) = -\frac{\mu^2}{2\pi}, \quad (9)$$

the free fermion result. Then, we ask if the two pressures cross at certain value of the chemical potential. They do at  $\mu = m/\sqrt{2}$ , reproducing the phase transition point predicted by the explicit leading large-N computation.

## VII. THE TBA IN NEXT TO LEADING ORDER

In our second paper we have gone one step further by generalizing the procedure to the next to leading order in  $1/N$  expansion. [2] The TBA equation is no longer trivial to solve but fortunately it can still be solved in a closed form. We skip all the technicalities and just quote the result. [2,19] The  $1/N$  correction to the free energy of the Gross-Neveu model can be given in a parametric form:

$$-P(\mu) = -\frac{m^2}{N\pi}[B^2 + \sinh^2 B - BShi(2B)] \quad (10)$$

$$\mu = m \cosh B + \frac{1}{N} [m \cosh B [Shi(2B) - 2B] - m \sinh B [Chi(2B) - \ln(\sinh 2B) - \gamma]] \quad (11)$$

where  $Shi(x)$  and  $Chi(x)$  are the hyperbolic integral functions defined by

$$\begin{aligned} Shi(x) &\equiv \int_0^x dt \frac{\sinh t}{t}, \\ Chi(x) &\equiv \gamma + \ln x + \int_0^x dt \frac{\cosh t - 1}{t}. \end{aligned} \quad (12)$$

The uncalculable constant, the vacuum energy density at zero chemical potential, was indeed calculated long time ago by Schönfeld. [21] With a bit of numerical computation the correction to the constant  $b$  can be written as

$$b = \frac{1}{4\pi} \left[ 1 - \frac{2.12}{3N} \right]. \quad (13)$$

Then, one can go through the exactly the same procedure as the leading order. We still obtain the free fermion result by taking the massless limit but with chemical potential with

1/N correction. It is what we expect because of the asymptotic freedom of the Gross-Neveu model. (See Ref. 2 for details.) The resulting correction to the critical point can be written as

$$\mu_c = \frac{m}{\sqrt{2}}[1 - \frac{0.47}{N}].$$

Therefore, it gives rise to about 20% correction to  $\mu_c$  at  $N=2$ . If it is expressed by critical dopant concentration  $y_c = 0.05$ , which is somewhat smaller than but still roughly agrees with the experimental value.

## VIII. CONCLUSION AND OUTLOOK

In this talk we have discussed how far one can proceed toward the thermodynamics of the Gross-Neveu model at zero temperature and finite background fermion density. At least in the 1/N expansion we have found that there is persistent first-order phase transition at a certain value of the chemical potential. Whether it survives in an exact treatment at  $N=2$  theory remains to be seen. However, we have argued that it is the case by relying on the following robust two features of the model: one is the chiral symmetry breaking at zero chemical potential as manifested in the kink spectrum which is known exactly by the method of factorizable S-matrix, and the other, the asymptotic freedom of the theory.

Is it possible to go beyond the large-N expansion? It is a very nontrivial question. In principle the answer is yes. Since all the S-matrix elements are known it should be possible to formulate the complete thermodynamics of the Gross-Neveu model. A more difficult but challenging question is whether the phase transition can be signaled solely within the framework of the TBA. We are now trying to answer (at least some of) these questions.

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